Tilt Grain-Boundary Effects in $S-$ and $D-$Wave Superconductors

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Abstract

We calculate the $s-$ and $d-$wave superconductor order parameter in the vicinity of a tilt grain boundary. We do this self-consistently within the Bogoliubov de Gennes equations, using a realistic microscopic model of the grain boundary. We present the first self-consistent calculations of supercurrent flows in such boundaries, obtaining the current-phase characteristics of grain boundaries in both $s-$wave and $d-$wave superconductors.

74.50.+r, 74.60.Jg, 74.80.-g

The debate over the superconducting order-parameter in the high T_c superconductors (HTSC) has been strongly contested, but has now been settled in favour of a $d-$wave pairing state [1,2]. The experiments by Tsuei *et al.* [3] and Wollman *et al.* [4] have been most conclusive, especially since they only depend on the phase of the order-parameter and not on the microscopic physics of the energy gap. Photoemission experiments [5] and the temperature depedence of the penetration depth [6] also strongly support the $d-$wave picture. However, some controversy still exists concerning possible $s-d$ mixing in the cuprates. In particular an s-wave component has been demonstrated to be induced at interfaces [7–9].

In interpreting the Tsuei *et al.* experiments it is essential to understand the superconducting characteristics of grain-boundary (GB) weak links in the cuprates. Understanding the effects of grain boundaries is also of importance for developing possible devices and other applications of high T_c superconductors. The Tsuei *et al.* experiments, especially the observations of π-junction behaviour, were consistent with the predictions of $d-$wave pairing interpreted using the Sigrist-Rice [10] model for the dependence of the critical current, I_c, on the grain boundary angles. On the other hand the values of I_c measured as a function of grain boundary angle show an almost exponential dependence on angle [11,12], unlike the cosine predicted by the Sigrist-Rice formula for $d-$wave pairing. In trying to explain these findings a number of different models of the interfaces have been studied. Tanaka and collegues [13] have looked at the (100) and (110) interfaces and also derived a Josephson current formula for $s/I/d$ and $d/I/d$ grain boundary structures. Barash *et al.* [14] have considered the temperature dependence of the critical current in d-wave junctions. Zhang considered 0^o, 45^o, and 90^o junctions [15]. Zhitomirsky and Walker [16] have also looked at the (110) interface to study the quasiparticle spectra and zero energy states (ZES). Beltzig *et al.* [17] showed that an induced $s-$wave component existed on the (orthorhombic) (110) boundary giving rise to a splitting in the ZES at a low enough temperature: the latter point they attribute to Time Reversal Symmetry Breaking (TRSB). The review on GBs by Prester [18] also highlights the possibility of them behaving as though each were an individual Joseph-

son Junction. Gurevich and Pashitskii argued that the near exponential depencence of I_c on angle was due to the formation of an insulating layer at the grain boundary, assosciated with the dislocation cores [19].

In this letter we address the effects of grain boundaries in both $s-$ and $d-$wave superconductors using a fully self-consistent solution of the Bogoliubov de Gennes (BdG) equations. We adopt a geometrically realistic model of the tilt grain boundary (GB), as shown in Fig.1. By solving the BdG equations in real space using the Recursion Method we are able to study such complex geometries, unlike earlier calculations which were limited to either simpler interfaces or planar junction models [20,15,21]. In consequence we can determine how the superconducting order-parameter (Δ), the charge density (n), and the quasi-particle local density of states (LDOS, $n(E)$) are affected by our GB. Further, by solving the BdG equations in a self-consistent manner we can apply phase-differences in Δ across the boundary and calculate the resulting supercurrent. By calculating the maximum current across the boundary we determine the critical current of the system.

For the purposes of this letter, we concentrate on the large angle grain-boundary (53.1^o), depicted in Fig.1. It consists of two square lattices butted together at some angle of misorientation and linked via a *percolation site*. Being periodic in the y direction we only have to undertake calculations for sites on two disimilar lines of atoms as shown in Fig. 1. For each line of sites we have to go 10 sites deep into the bulk before the order parameter has recovered to its bulk value. For some bonds across the GB the interatomic spacing is less than the bulk spacing. For these bonds we assume that the value for the hopping between sites i and j (t_{ij}) can be calculated by assuming a simple linear form for the hopping-integral, i.e.

$$t_{ij} = -\frac{\sqrt{2} - r_{ij}}{\sqrt{2} - 1}, \quad 0 \leq r_{ij} \leq \sqrt{2} \tag{1}$$

and is zero otherwise. For the geometry of our GB (Fig.1) every site will have a *connectivity* of 4.

We consider the following two attractive Hubbard models:

$$H = \sum_{<i,j>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{2}$$

$$H = \sum_{<i,j>,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + h.c. + U \sum_{<i,j>} n_{i} n_{j} \tag{3}$$

with $U < 0$ and $n_i = n_{i\uparrow} + n_{i\downarrow}$. Here U is the usual BCS pairing-potential, defined as being a negative constant within a cutoff energy range of $\pm E_c$ either side of the Fermi energy, after which its value is zero. Eq.2 will be refered to as 'local', giving rise to $s-$wave pairing and Eq.3 will be termed 'non-local' giving $d-$wave pairing. By making the Bogoliubov canonical- transformation we diagonalise the Hamiltonian and arrive at the Bogoliubov-de Gennes equations

$$\sum_{j} \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta^{\star}_{ij} & -H^{\star}_{ij} \end{pmatrix} \begin{pmatrix} u^{n}_{j} \\ v^{n}_{j} \end{pmatrix} = E_n \begin{pmatrix} u^{n}_{i} \\ v^{n}_{i} \end{pmatrix} \tag{4}$$

where $H_{ii} = (-\mu + \frac{1}{2} U n_{ii})$ and $H_{ij} = t_{ij}$ (local), or, $H_{ii} = -\mu$ and $H_{ij} = t_{ij} + \frac{1}{2} U n_{ij}$ (non-local). Here μ is the chemical potential, u^{n}_{i} and v^{n}_{i} are the particle and hole amplitudes on site i associated with an eigenenergy E_n, and n_{ij} is the appropriate charge density (defined below). To solve these equations we employ the Recursion Method [22], and together with the methods employed in Martin and Annett [23], we obtain a matrix continued-fraction for the Green functions. This continued-fraction is evaluated exactly to 50 levels after which its elements vary in a predictable manner and therefore can be extrapolated for a futher 1500 levels say.

We are interested in evaluating the local quasi-particle density of states, the local and non-local charge densities ($n_{ii} = \sum_{\sigma} \langle c^{\dagger}_{i\sigma} c_{i\sigma} \rangle$ and $n_{ij} = \sum_{\sigma} \langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle$ respectively), and the local and non-local order-parameters ($\Delta_{ii} = U \langle c_{i\uparrow} c_{i\downarrow} \rangle$ and $\Delta_{ij} = U \langle c_{i\uparrow} c_{j\downarrow} \rangle$ respectively). These quantities may be found from the Green functions, expressions for which have already been given elsewhere [23]. In the calculations that follow we make a BCS cutoff of $U = -3.5t$, have a temperature, T, of $T = 0.01t$, and $E_c = 3.0t$. Iterating the equations for charge-densities and order-parameters, with the BdG equations, we generate self-consistent solutions. So as not to direct the final SC solution into a local energy minimum, we set the

order-parameter to zero at the beginning of the calculation on those sites closest in proximity to the boundary. We say self-consitency has been achieved when the Hartree-Fock term and the order-parameter change by less than a predefined margin between iterations. For the $s-$wave case, we can reach 0.5% s.c. typically between 10 or 20 iterations, whereas for the $d-$wave it usually takes over 200 iterations.

By imposing a phase-difference φ in the order-parameter between the two bulk regions we may now generate current-flow across the GB. We initially make the Peierls substitution for t_{ij}, ($t_{ij} \rightarrow t_{ij}e^{-ieA_{ij}/\hbar}$, A_{ij} being the integral of the vector-potential between sites i and j), in Eq.2 and 3, and use the definition $I_{ij} = \langle \frac{\partial H}{\partial A_{ij}} \rangle$, to obtain [24]

$$I_{ij} = \frac{t_{ij}e}{\hbar} \Re \Big[\frac{1}{\pi} \int_{-\infty}^{+\infty} [G_{ij}(E + \imath\eta) - G_{ij}(E - \imath\eta)] e^{-ieA_{ij}/\hbar} f(E) dE \Big] \tag{5}$$

$f(E)$ being the Fermi-Dirac function. By a suitable choice of gauge we can immediately set $A_{ij} = 0$ everywhere.

When applying phase-differences in Δ across a GB it is instructive to note how Δ changes due to the self-consitency, and also observe how the local densities of states and the Hartree-Fock term alter. Fig.2 shows the results for the $s-$wave case. Figs.2(a) and 2(b) show the evolution of $|\Delta_{ii}|$ across the GB on both the lower (a) and upper (b) lines of SC sites at $\varphi = 0^o$ (full line) and also $\varphi = 180^o$ (dotted line). The GB obviously has a perturbing effect on the system but note that $|\Delta_{ii}|$ is not depressed on the percolation site ($x = 0$) for $\varphi = 0^o$. Infact $|\Delta_{ii}|$ is almost constant as φ is varied; except for $\varphi = 180^o$ where $|\Delta_{ii}| = 0$ on the percolation site and is strongly reduced nearby. Note also the small Friedel-like oscillations in $|\Delta_{ii}|$ near the GB. Fig.2(c) shows how the order parameter phase, $arg(\Delta_{ii})$, varies as a function of x co-ordinate through the GB for the $\varphi = 30^o$ case. For the 180^o case we just have a step function with arbitrary phase associated with the percolation site since $|\Delta_{ii}| = 0$. For all other phase differences, the phase as a function of x goes as $(\varphi/2)\tanh(x/d)$ where φ is the bulk phase difference across the GB and d is a characteristic length scale which we find to be $d = 3.5$ for our parameters. Also, this equation holds for both SC lines. Finally,

in Fig.2(d) we show the local density of states on the percolation site at $\varphi = 0^o$ (full line) and at $\varphi = 180^o$ (dotted line). At 0^o we have the usual BCS-like gap around the Fermi energy. This persists through all our calculated phase-differences except at 180^o where the gap is suddenly filled in with various resonant states. Although not presented here we note that the Hartree-Fock term $\frac{1}{2}Un_{ii}$ shows the same (enhanced) values on both lines of SC sites at different phase-differences.

Now consider the $d-$wave case. Because each site has four bonds with order parameters Δ_{ij} we can calculate the 'net' $d-$wave contribution at a particular site by considering $\Delta_i^d = \sum_{j=1,4}(-1)^j\Delta_{ij}$ Similary, the extended$-s$ component is given by $\Delta_i^s = \sum_{j=1,4}\Delta_{ij}$ and will be finite near the boundary because of the broken crystallographic symmetry. A minor difficulty now arises when discussing the $d-$wave scenario. In the definition of Δ_i^d we must choose a convention for the direction of the positive and negative lobes of the $d-$wave function. For GB angles close to 45^o, such as in Fig.1, there is an ambiguity in defining the relative orientations of the order parameter lobes either side of the GB. The convention we have chosen is indicated in Fig.1. In this case the current-phase relationship, $I(\varphi)$, is similar for both $s-$wave and $d-$wave cases. For this choice the $d-$wave order parameter is zero on the percolation site, $x = 0$, for zero phase difference, Fig.3(a), unlike the $s-$wave case of Fig.2(a). Using our definition of phase-differences we find a maximum $d-$wave contribution at 180^o on the lower line of SC sites (dotted line), which decreases with phase-difference, down to 0^o (full line) where $|\Delta_{x=0}^d| = 0$. The upper line of SC sites (Fig.3(b)) shows the same qualitative form for Δ_d as for the local $s-$wave case. At 0^o we find maximum extended$-s$ component on the precolation site (full line in Fig.3(c)), decreasing with increasing phase-difference until at 180^o we have minimum extended$-s$ contribution (dotted line). Fig.3(d) illustrates how the extended$-s$ component evolves on the upper line of SC sites at either phase difference. Thus we conclude that the extended$-s$ and the $d-$wave components are in competition such that the extended$-s$ component is maximised at the detriment of the $d-$wave and vice versa.

Fig.4 shows the calculated currents in both the local $s-$wave and non-local $d-$wave

cases. To calculate the current (using Eq.5) we have to consider the flow across all possible routes in just one cell of our sample. In calculating currents it is essential to check current conservation: this is only guaranteed from a self-consistent solution. Here, we find conservation obeyed to within 0.01%. Consider the $s-$wave intially: the variation of current with phase-difference,φ, is plotted in Fig.4 (solid line) where the values for phase difference range from 0^o to $+180^o$. It is immediately clear that the current is not sinusoidal in φ but instead shows a sharp step at 180^o. The remainder is roughly that of a saw-tooth albeit with some saturation. The step at $\pm 180^o$ can be attributed to resonant states entering the gap [25,26]. Fig.2(d) compares the local quasi-particle density of states at $\varphi = 0^o and 180^o$ confirming the presence of resonant midgap states at 180^o.

Our calculations for the d-wave current are presented in Fig.4 (dashed line). Again it is approximately a sawtooth. The slope $\frac{\partial I}{\partial \varphi}$ is also positive, and consequently this GB cannot be classified as a π-junction: this is consistent with the Sigrist-Rice formula for this geometry. Fogelström and Yip [28] note that in certain geometries it is also possible to have a vanishing current at phase-differences other than integer multiples of π, and this they attribute to time reversal symmetry breaking (this has been reported in Il'ichev [27]). Fig.4 shows no such evidence and therefore we conclude that the symmetric grain-boundary does not have TRSB.

In conclusion we have developed a real-space method for determining how the order parameter and supercurrents change with phase-difference across a realistic interface in a superconductor. In this letter we have considered a large-angle symmetric tilt grain-boundary and considered the local $s-$wave and non-local $d-$wave pairing symmetry in the order-parameter on an equal footing. We have calculated the LDOS, Hartree-Fock terms, order parameter and current all self-consistently. By imposing a phase differnce, φ, across the junction we calculated the supercurrent $I(\varphi)$. We found, for both $s-$wave and $d-$wave that $I(\varphi)$ is non-sinusoidal but exhibits a saw-tooth like behaviour which can be attributed to a sudden filling-in of the energy gap at $\varphi = 180^o$. Further, we note no time reversal symmetry breaking or π-junction behaviour in the $d-$wave case.

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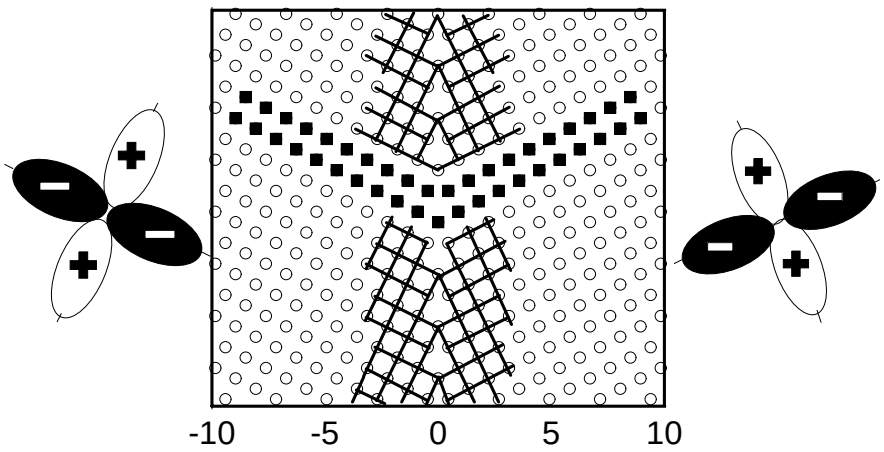
FIGURES

FIG. 1. *The symmetric model tilt grain-boundary. By periodicity, we carry out self-consistent calculations on two lines of sites (highlighted) which are then mirrored onto similar sites in the rest of the sample. Also shown is our definition of a d-wave* 0^o *phase difference across the boundary (see text).*

FIG. 2. *a) order-parameter on lower line of SC sites at* 0^o *(full line) and* 180^o *(dotted line). The latter goes to zero on the percolation site (*$x = 0$*), b)same as a) but for upper line of SC sites, c) self consistently determined evolution of the order-parameter phase on going through the GB for a* 30^0 *phase difference, d) Quasiparticle local density of states at* 0^o *phase difference (full line) and at* 180^o *(dashed line).*

FIG. 3. *The contributions to the superconducting order-parameter (*$d-$*wave) on going through the boundary. The x coordinate is plotted on the horizontal axis. Full line refers to* 0^0 *phase difference, dashed refers to* 180^0*: a) d-wave on lower line b) d-wave on upper line c) extended-s on lower line d) extended-s on upper line*

FIG. 4. *The supercurent versus phase-difference in the order-parameter between the two bulk regions for the s-wave and d-wave cases.*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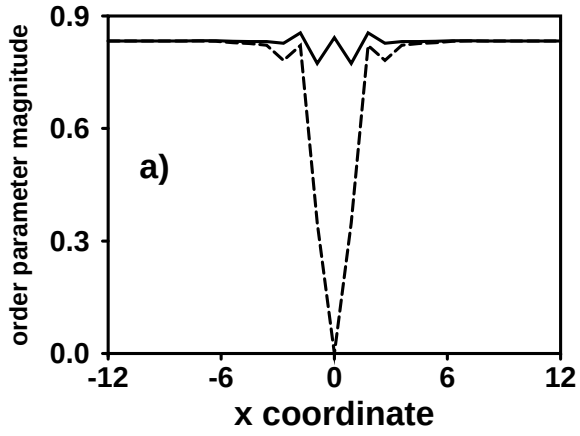
-5
0
5
10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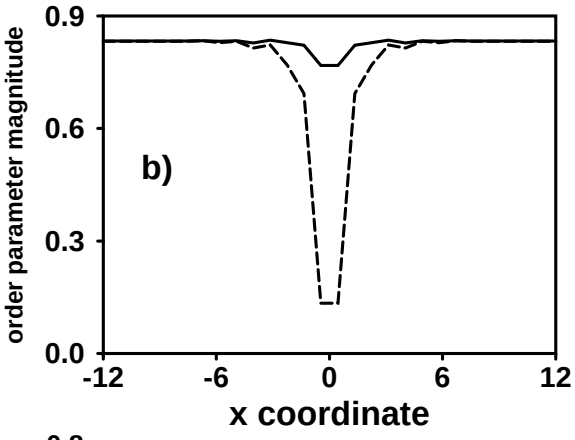
0.6
0.3
0.0
a)
-12
-6
0
6
12
x coordinate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0.0
b)
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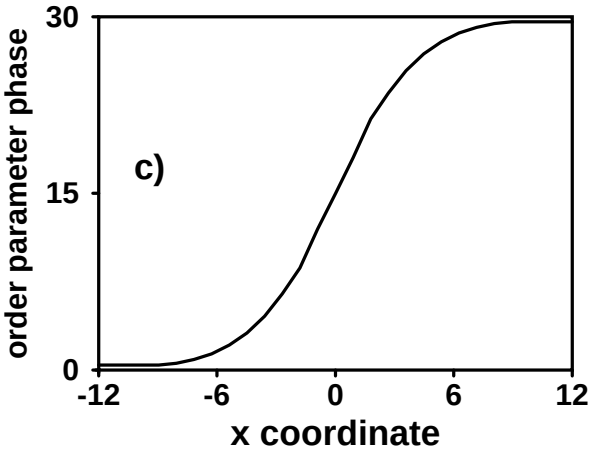
0
6
12
x coordinate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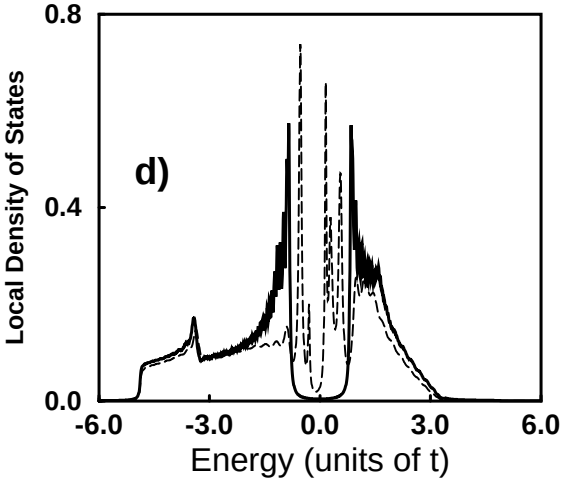
15
0
c)
-12
-6
0
6
12
x coordinate


Local Density of States
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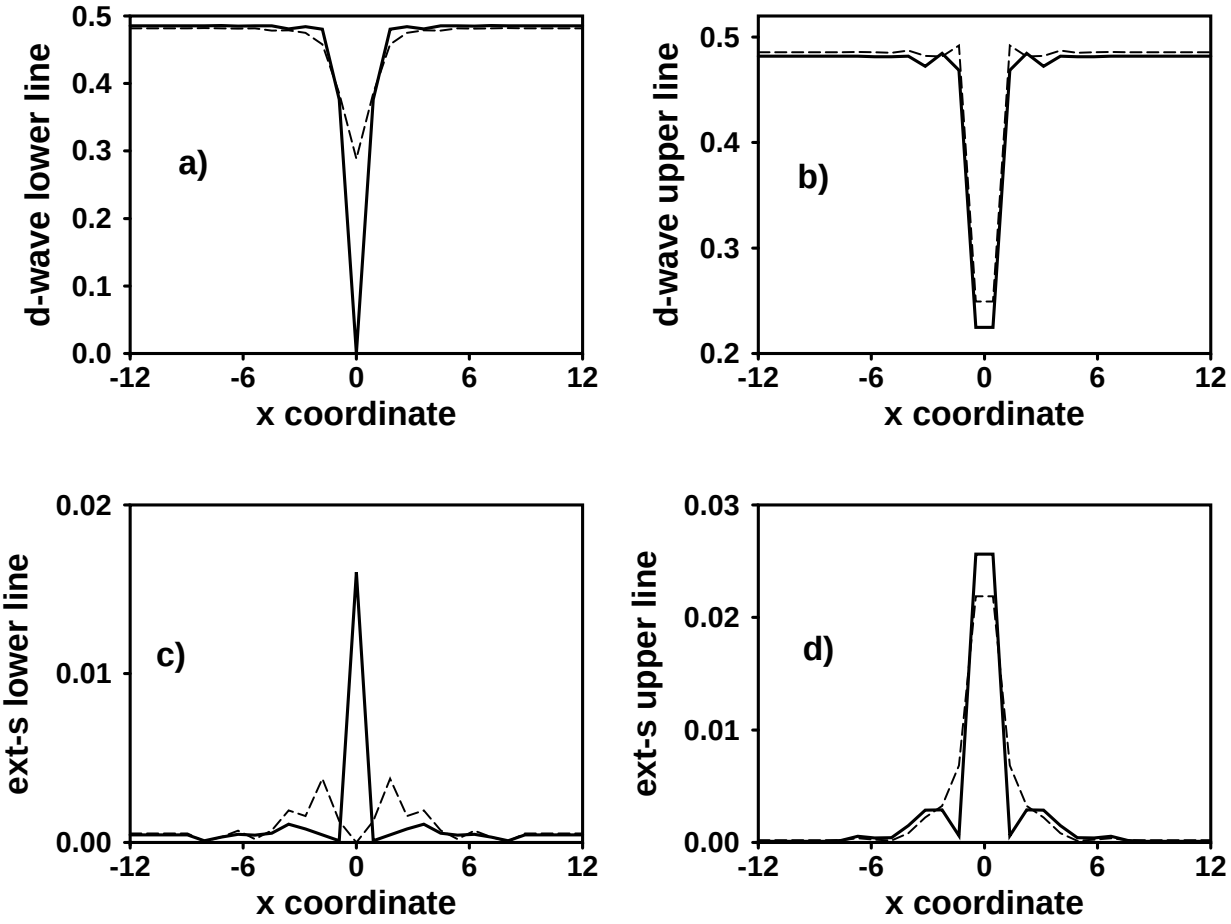
0.4
0.0
d)
-6.0
-3.0
0.0
3.0
6.0
Energy (units of t)


a)
b)
c)
d)
d-wave lower line
d-wave upper line
ext-s lower line
ext-s upper line
x coordinate
0.5
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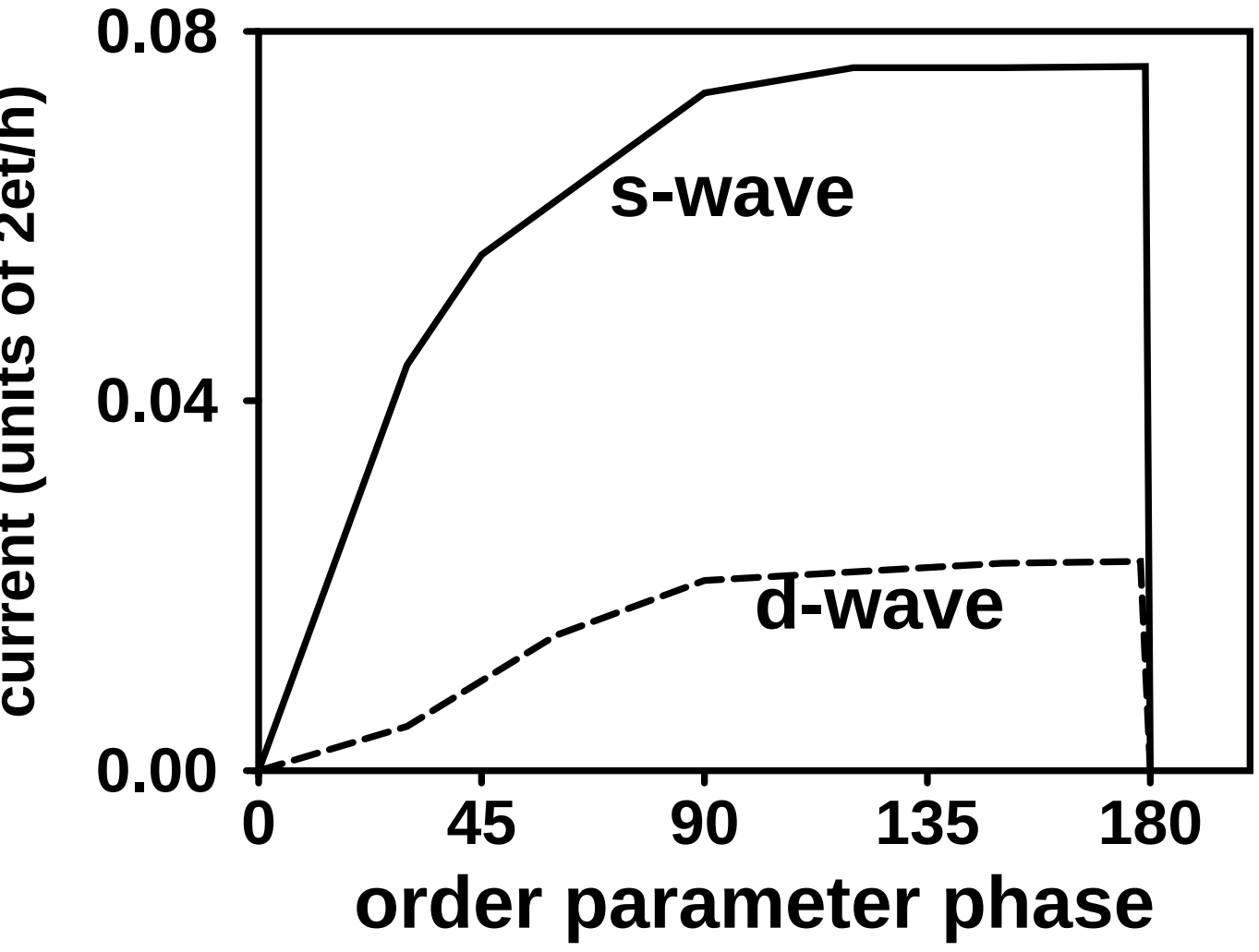
0.1
0.0
0.02
0.01
0.00
0.03
-12
-6
0
6
12


0.08
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0.00
current (units of 2et/h)
s-wave
d-wave
0
45
90
135
180
order parameter phase